

US EPA ARCHIVE DOCUMENT

HIERARCHICAL (MULTI-SCALE) MODELING FRAMEWORK

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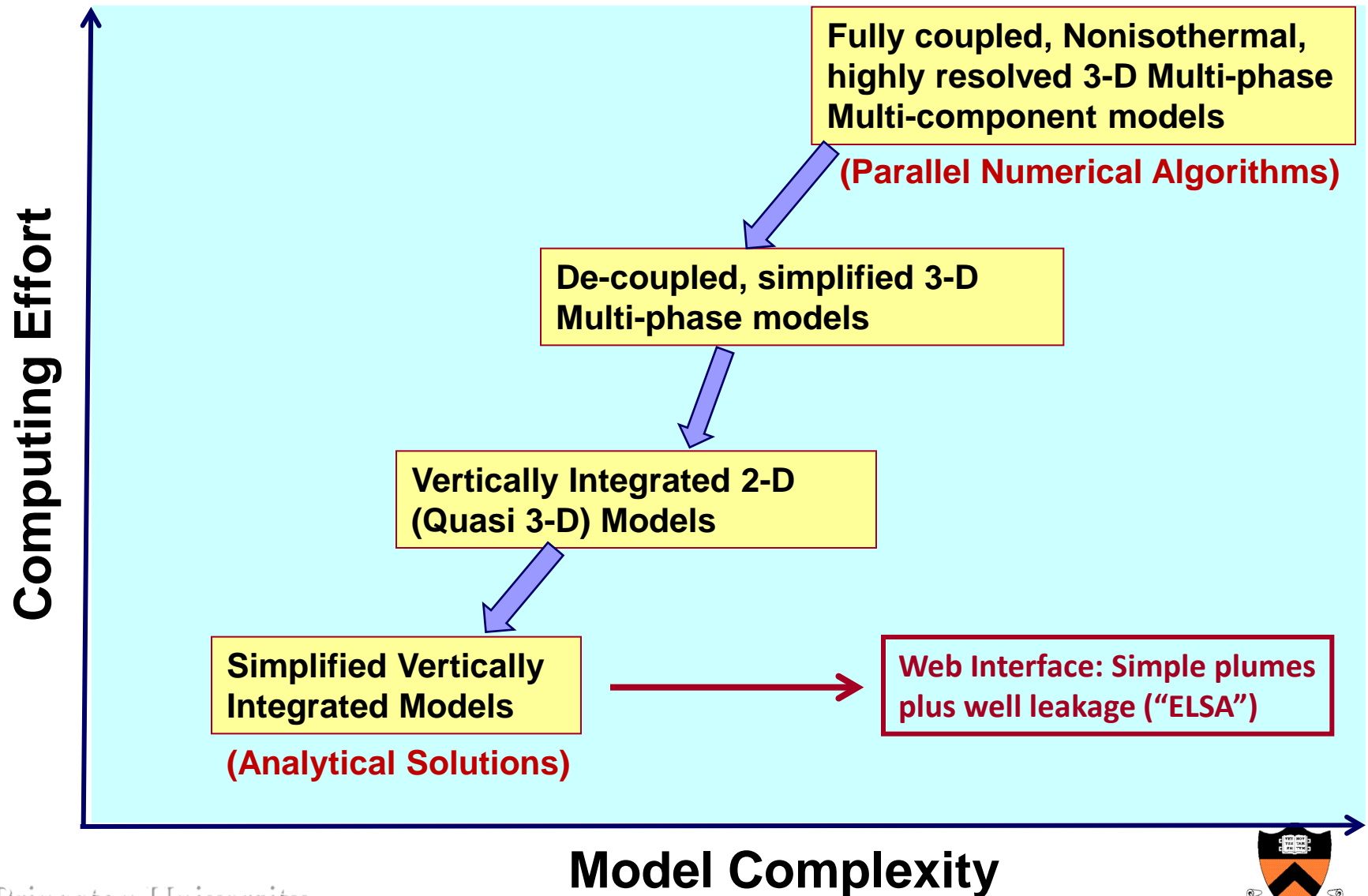


OUTLINE

- Model Complexity and Practical Models
- Simple Vertical Equilibrium Models
- Multi-scale Models
 - Vertical Integration and Vertical Reconstruction
 - Dissolution and Convective Mixing
 - Concentrated features / leakage pathways
- Example Calculations
- Final Remarks

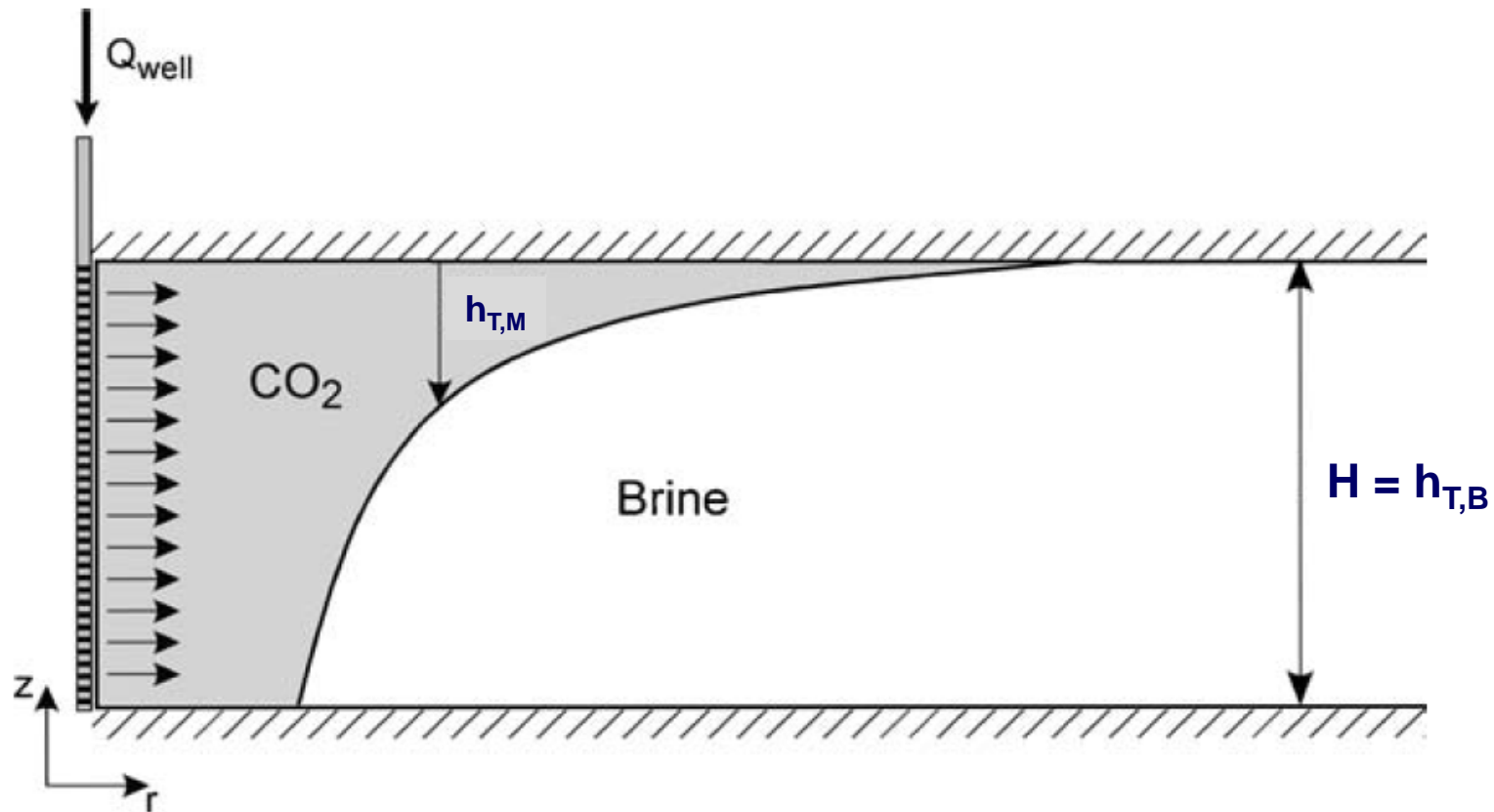


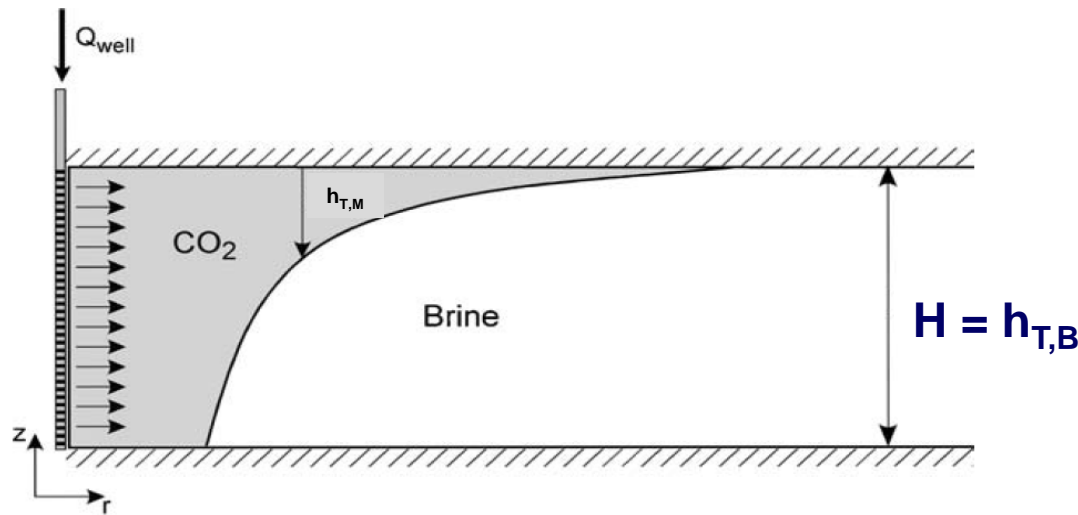
A HIERARCHY OF MODELS



SIMPLEST ANALYTICAL SOLUTION

- Horizontal, homogeneous formations.
- Constant injection rate in a single vertical well.
- Vertical Equilibrium and Sharp Interface



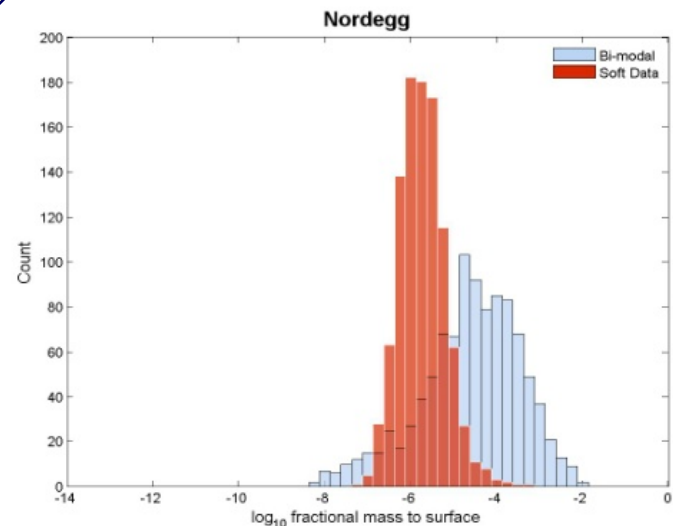
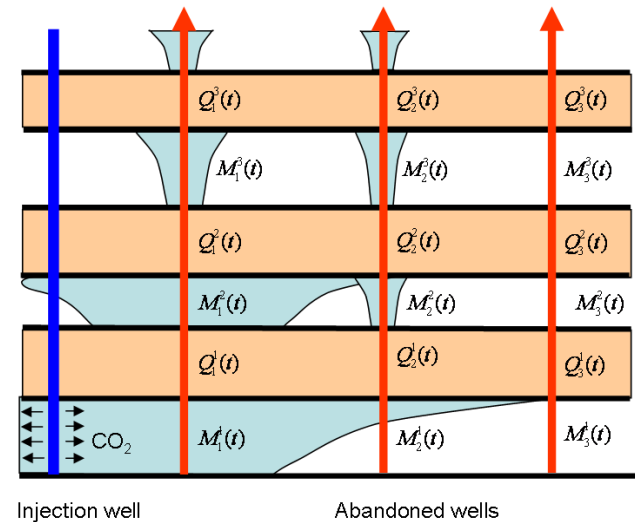
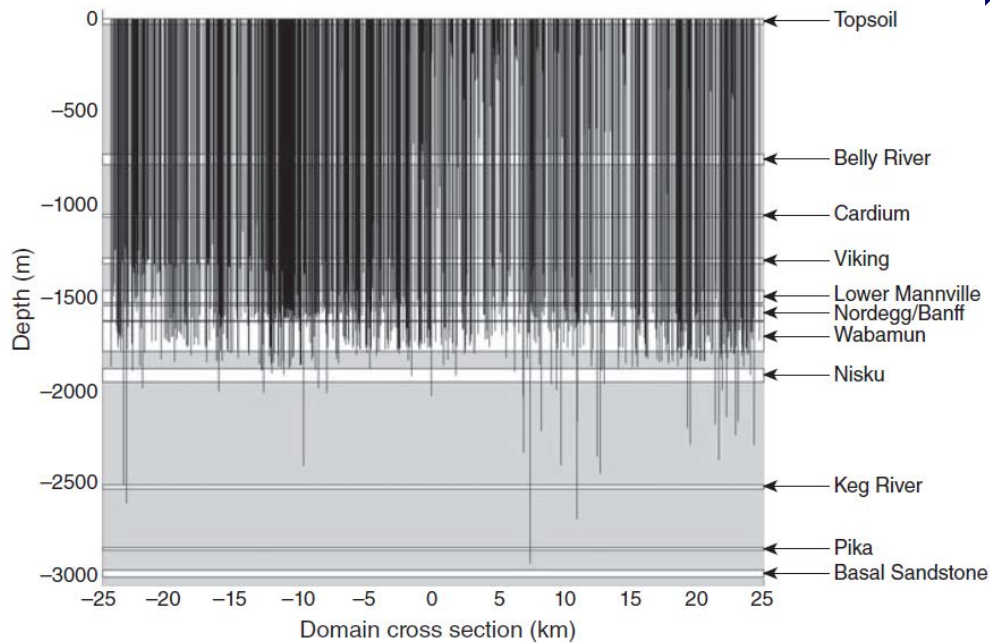
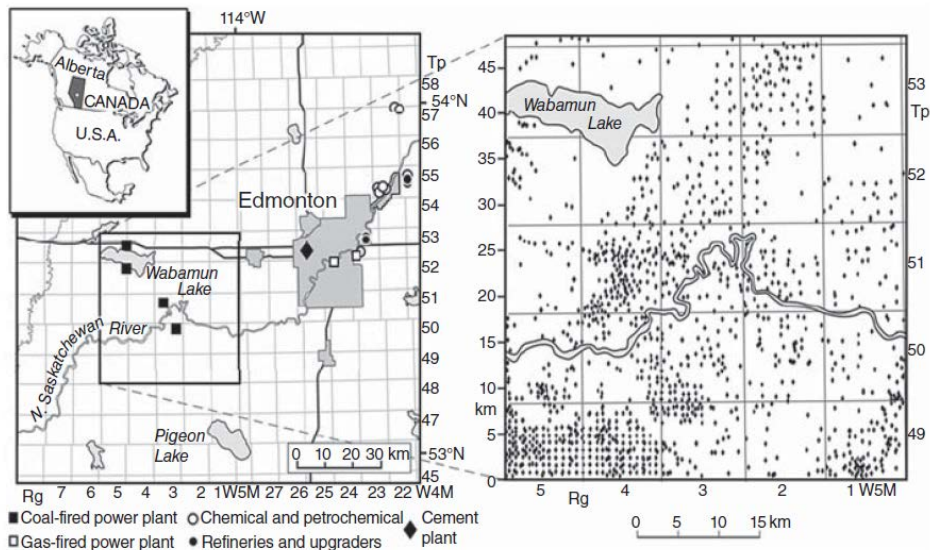


$$\chi \equiv \frac{\pi \Phi r^2}{Q_{\Sigma} t}$$

$$\frac{S_c(\chi)}{S_{c,T}} = \frac{h_{T,M}}{h_{T,B}} = \begin{cases} 0 & \text{if } S_{c,T}\chi \geq \lambda \\ \frac{1}{\lambda - 1} \left(\sqrt{\frac{\lambda}{S_{c,T}\chi}} - 1 \right) & \text{if } \lambda^{-1} < S_{c,T}\chi < \lambda \\ 1 & \text{if } 0 < S_{c,T}\chi \leq \lambda^{-1} \end{cases}$$

$$\Gamma = 2 \frac{\pi K \Lambda'_b \Delta_{\alpha} \rho g h_{T,B}}{Q_{\Sigma}} (< 0.1)$$





(See: Celia et al., 2011)



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The New York Times - Breaking News, W... <http://monty.princeton.edu/CO2interface/>

monty.princeton.edu/CO2interface/

ELSAWeb Simple Model Complex Model

Display: System Schematic | Plume Evolution | Pressure

SIMULATION PARAMETERS

Click on a parameter value below to edit.
Roll over parameter name for more info.

Domain		
Outer Radius:	50000	[m]

Injection Aquifer General Properties		
Top Depth:	1500	[m]
Thickness:	50	[m]
Permeability:	5e-14	[m ²]
Brine Residual Sat:	0	[L ³ /L ³]
CO ₂ Relative Perm:	1	[m ² /m ²]
Porosity:	0.15	[L ³ /L ³]
Compressibility:	4.2e-10	[Pa ⁻¹]

Injection Aquifer Fluid Properties		
Parameters below can be edited manually, or click the calculator above to calculate densities and viscosities based on a temperature and pressure gradient.		
CO ₂ Density:	479	[kg/m ³]
CO ₂ Viscosity:	0.0000395	[Pa.s]
Brine Density:	1045	[kg/m ³]
Brine Viscosity:	0.0002535	[Pa.s]

Injection Well		
Injection Rate:	1	[Mt/yr]

Analysis		
Simulation Time:	50	[years]

Run Simulation Reset Parameters

VISUALIZATION

Plume Evolution

Depth [m]

Distance [km]

Time: 35.1 years.



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monty.princeton.edu/CO2interface/index_complex.html

ELSAWeb Simple Model Complex Model

Display: System Schematic | Plume Evolution | Pressure

SIMULATION PARAMETERS

Click on a parameter value below to edit.

Domain		
Outer Radius:	50000	[m]

Injection Aquifer		
Top Depth:	2000	[m]
Thickness:	50	[m]
Permeability:	5e-14	[m ²]
Brine Residual Sat:	0	[L ³ /L ³]
CO ₂ Relative Perm:	1	[m ² /m ²]
Porosity:	0.15	[L ³ /L ³]
Compressibility:	4.2e-10	[Pa ⁻¹]

Overlying Aquifer		
Top Depth:	1500	[m]
Thickness:	50	[m]
Permeability:	5e-14	[m ²]
Brine Residual Sat:	0	[L ³ /L ³]
CO ₂ Relative Perm:	1	[m ² /m ²]
Porosity:	0.15	[L ³ /L ³]
Compressibility:	4.2e-10	[Pa ⁻¹]

Fluid Properties		
Parameters below can be edited manually, or click the calculator above to calculate densities and viscosities based on a temperature and pressure gradient.		
Injection Aquifer		
CO ₂ Density:	479	[kg/m ³]
CO ₂ Viscosity:	0.0000395	[Pa.s]
Brine Density:	1045	[kg/m ³]

VISUALIZATION

Plume Evolution

Depth [m]

Distance [km]

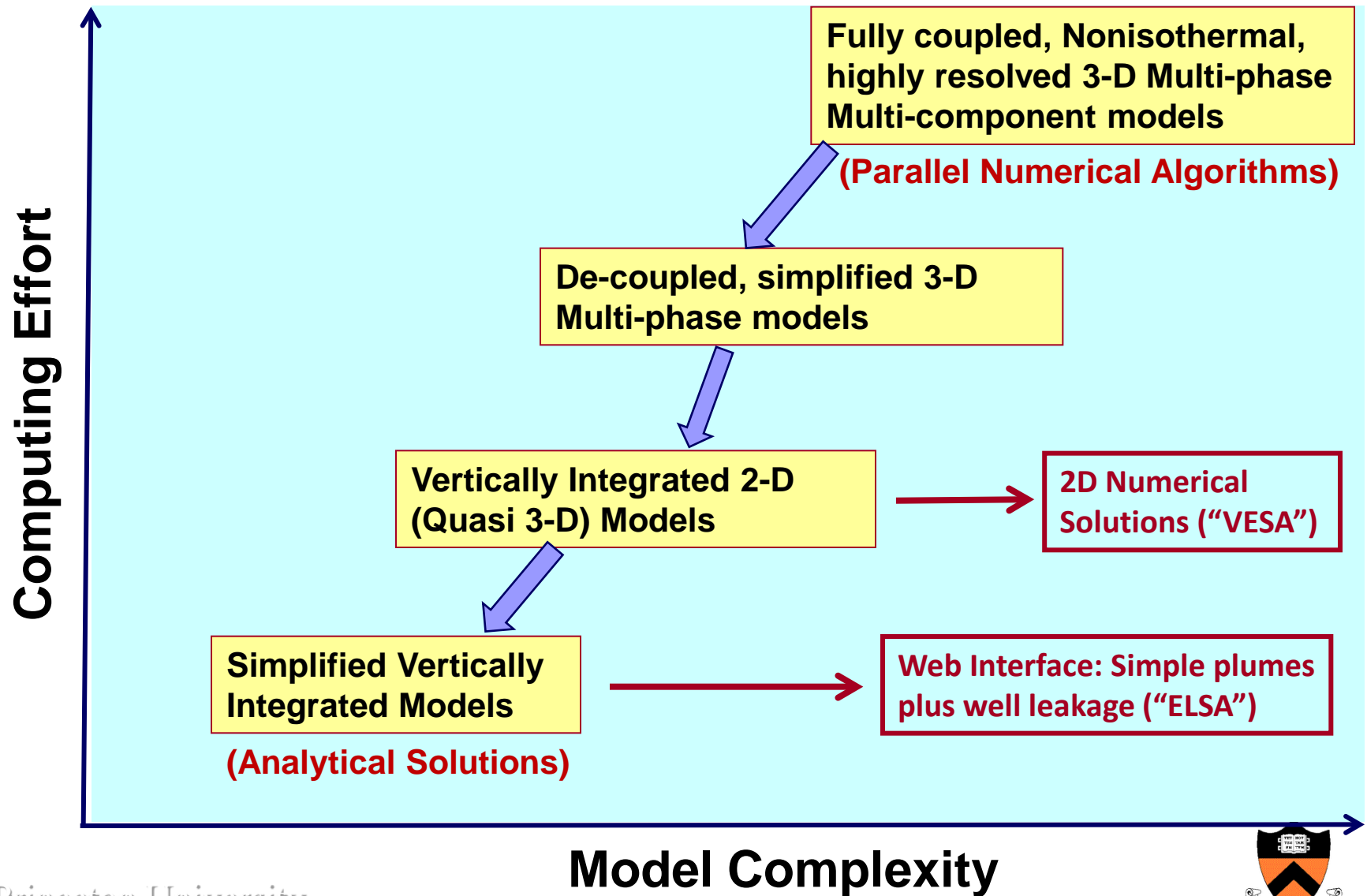
Time: 45.3 years.

Start

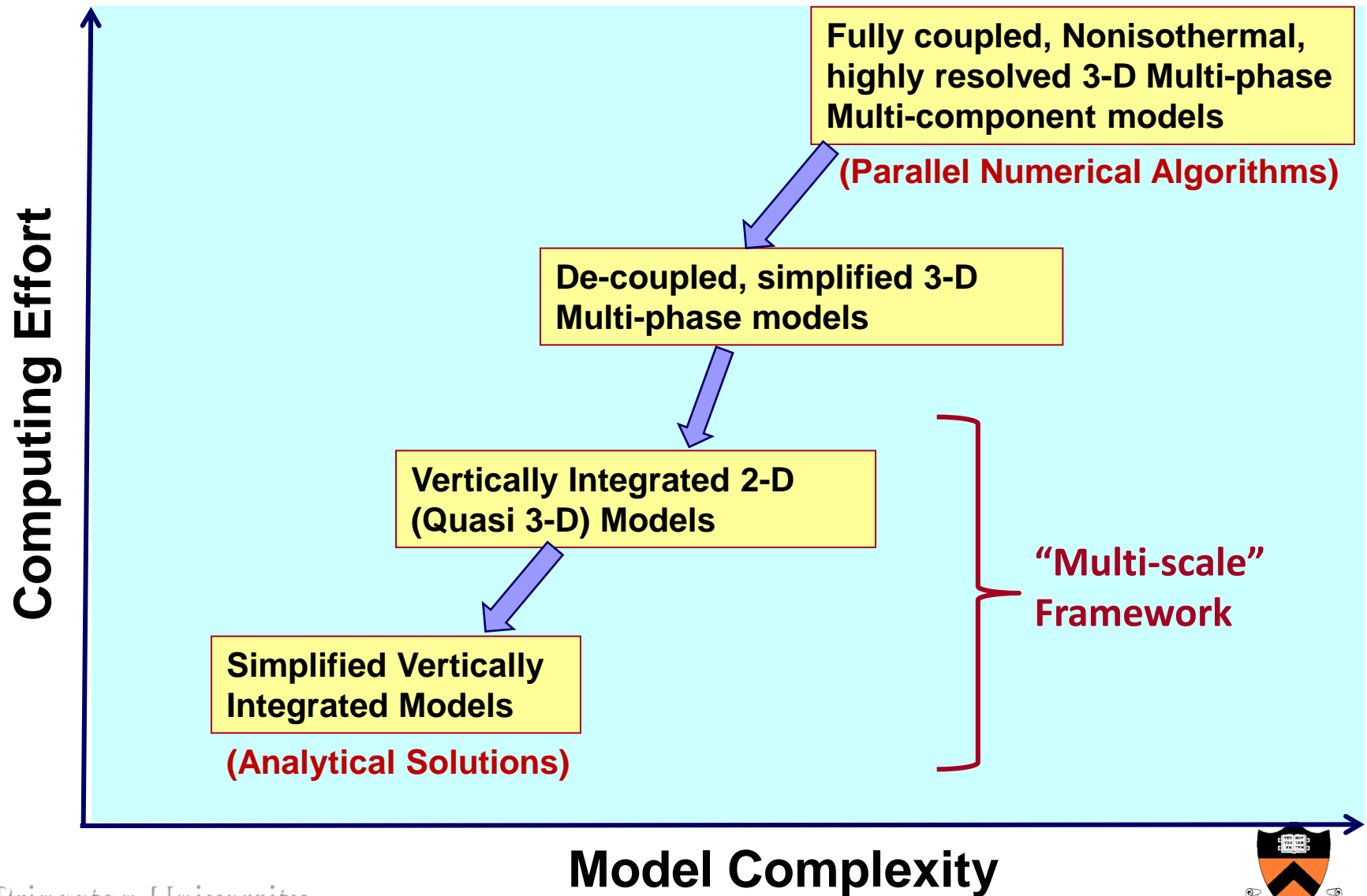
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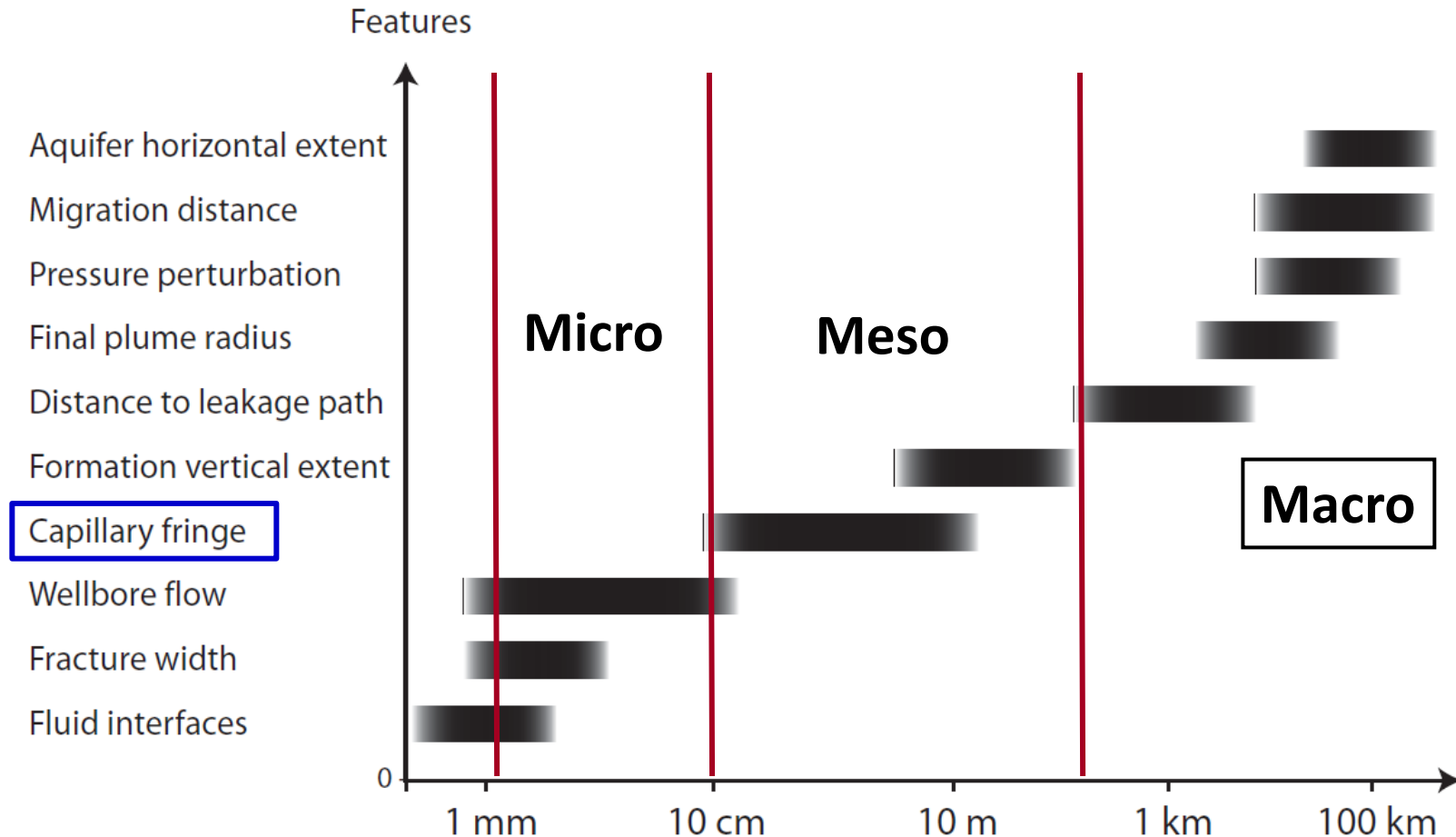
A HIERARCHY OF MODELS



A HIERARCHY OF MODELS



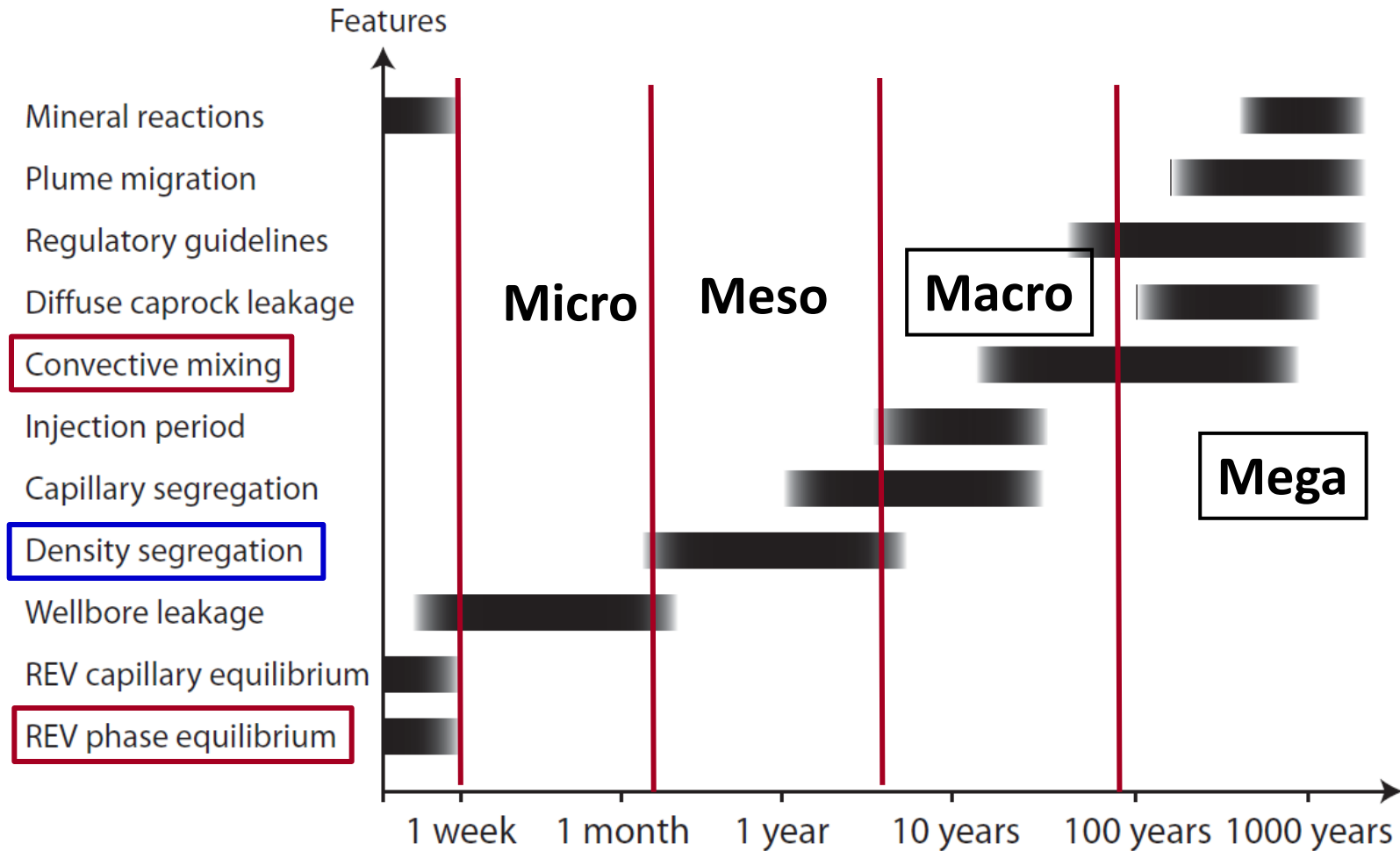
SPATIAL SCALES



(See: Nordbotten and Celia, 2012)



TEMPORAL SCALES



(See: Nordbotten and Celia, 2012)

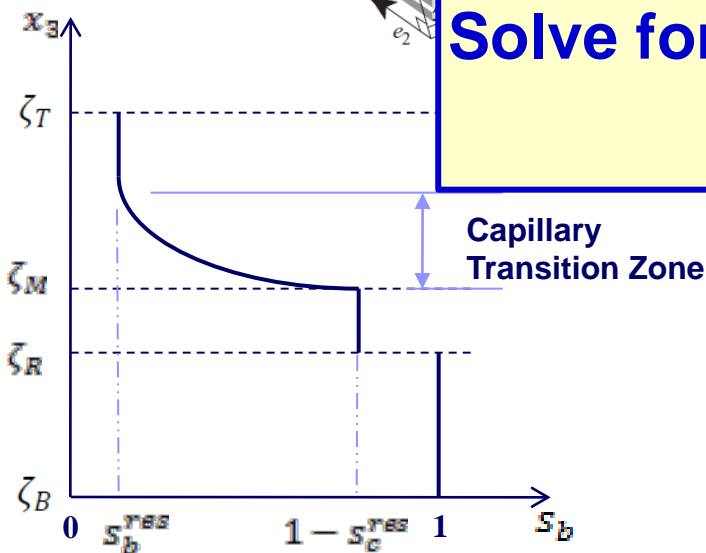
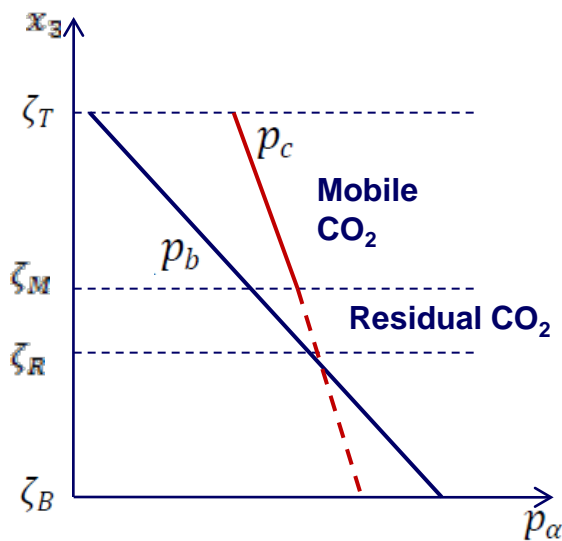
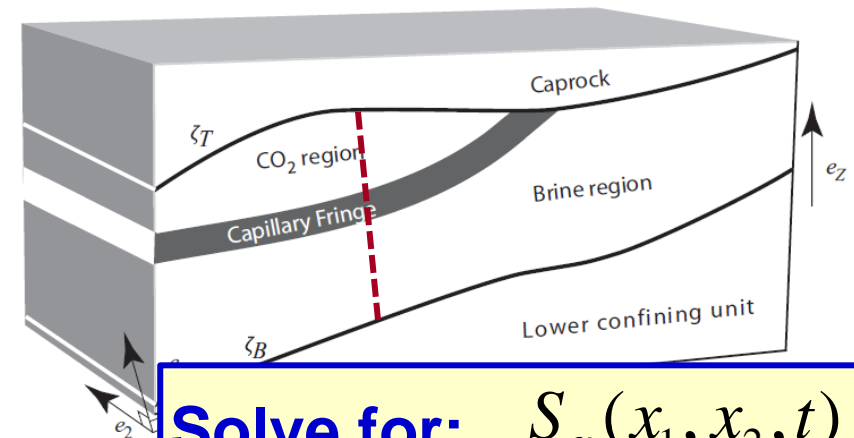


Vertically Integrated Models (VESA)

Key Assumption: *Density segregation* has occurred ($t^* \ll T$).

Simplest Case: Zero velocity along x_3 (“vertical equilibrium” or “Dupuit assumption”)

$$t^* \sim f(\Delta\rho, k_z, H, k_{rel}^*)$$



Solve for: $S_\alpha(x_1, x_2, t)$
 $P_\alpha(x_1, x_2, t)$

Vertically Integrated Models

$$\Phi \frac{\partial S_\alpha}{\partial t} - \nabla_{||} \cdot (K \Lambda_\alpha (\nabla_{||} P_\alpha - \varrho_\alpha \mathbf{G})) = \Upsilon_\alpha$$

$$\Phi = \int_{\zeta_B}^{\zeta_T} \varphi dx_3 \quad S_\alpha = \frac{1}{\Phi} \int_{\zeta_B}^{\zeta_T} \varphi s_\alpha dx_3$$

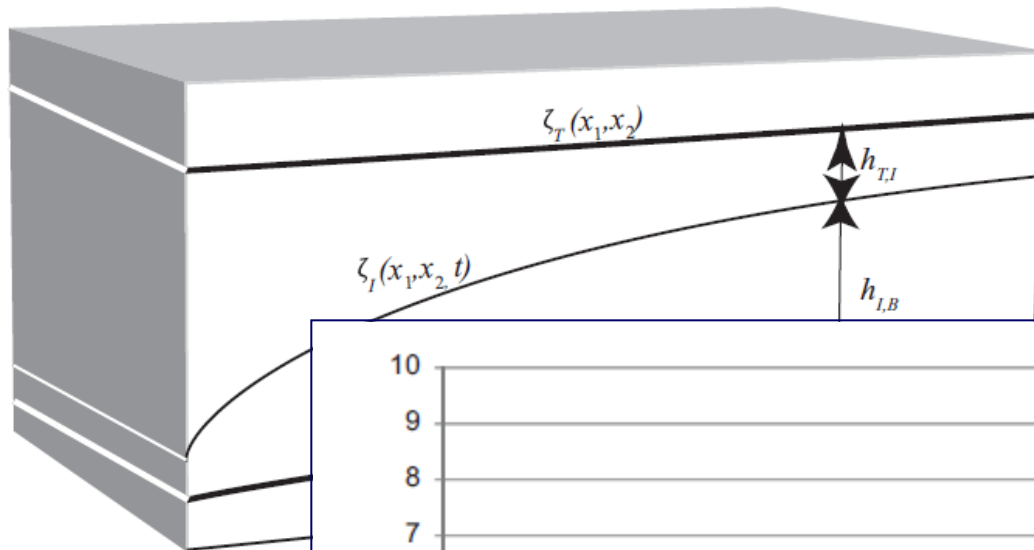
$$K = \int_{\zeta_B}^{\zeta_T} k_{||} dx_3 \quad \Lambda_\alpha = K^{-1} \int_{\zeta_B}^{\zeta_T} k_{||} \lambda_{\alpha,||} dx_3 \quad \mathbf{G} = \mathbf{e}_{||} \cdot \mathbf{g} + (\mathbf{g} \cdot \mathbf{e}_3) \nabla_{||} \zeta_P$$

P_α is the phase pressure at a chosen datum elevation ($x_3 = \zeta_P$)

1. **Solve coarse equation for** $S_\alpha(x_1, x_2, t), P_\alpha(x_1, x_2, t)$
2. **Reconstruct** $\hat{s}_\alpha(x_1, x_2, x_3, t), \hat{p}_\alpha(x_1, x_2, x_3, t)$
3. **Update mobilities** $\hat{\lambda}_\alpha(x_1, x_2, x_3, t), \Lambda_\alpha(x_1, x_2, x_3, t)$



Sharp Interface Assumption



Capillary Transition Zone negligible

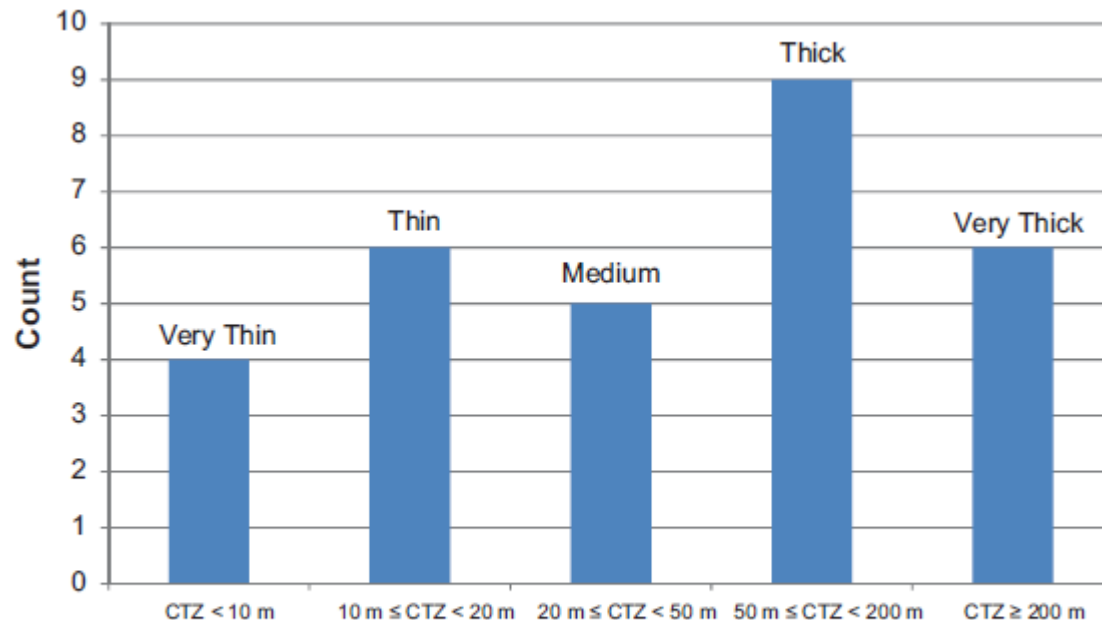
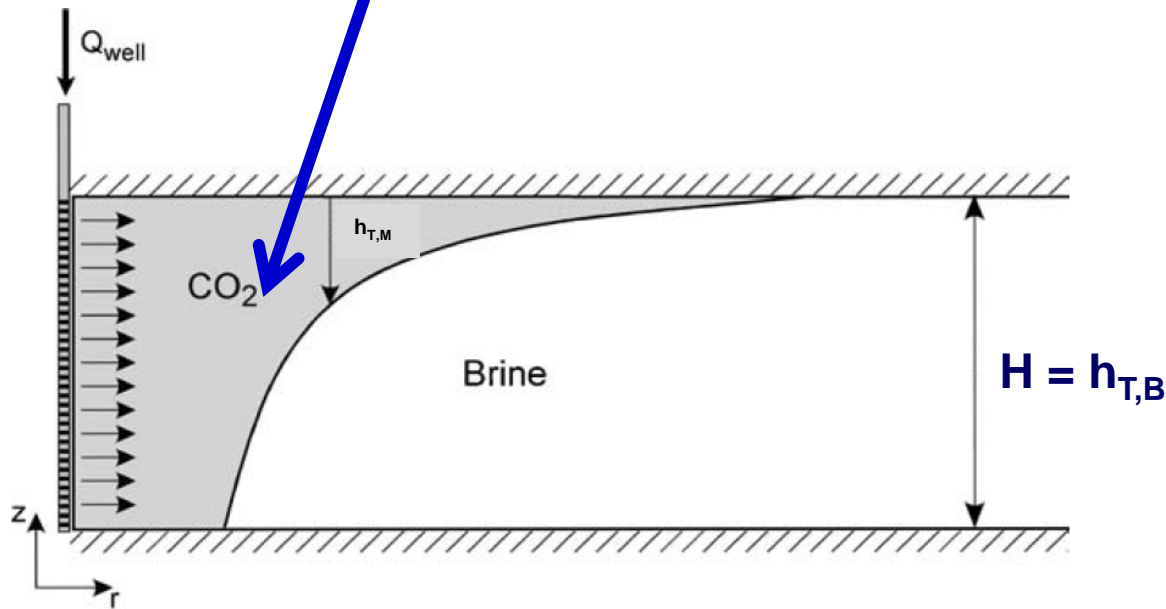


Fig. 3. Capillary Transition Zone (CTZ) thicknesses reported in Table 2 grouped into five typical aquifer thickness categories.

(See: Court et al., 2012)

Dissolution and Geochemistry

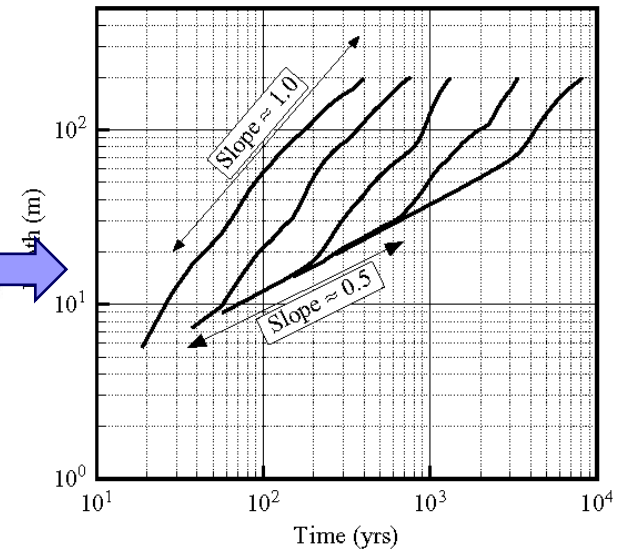
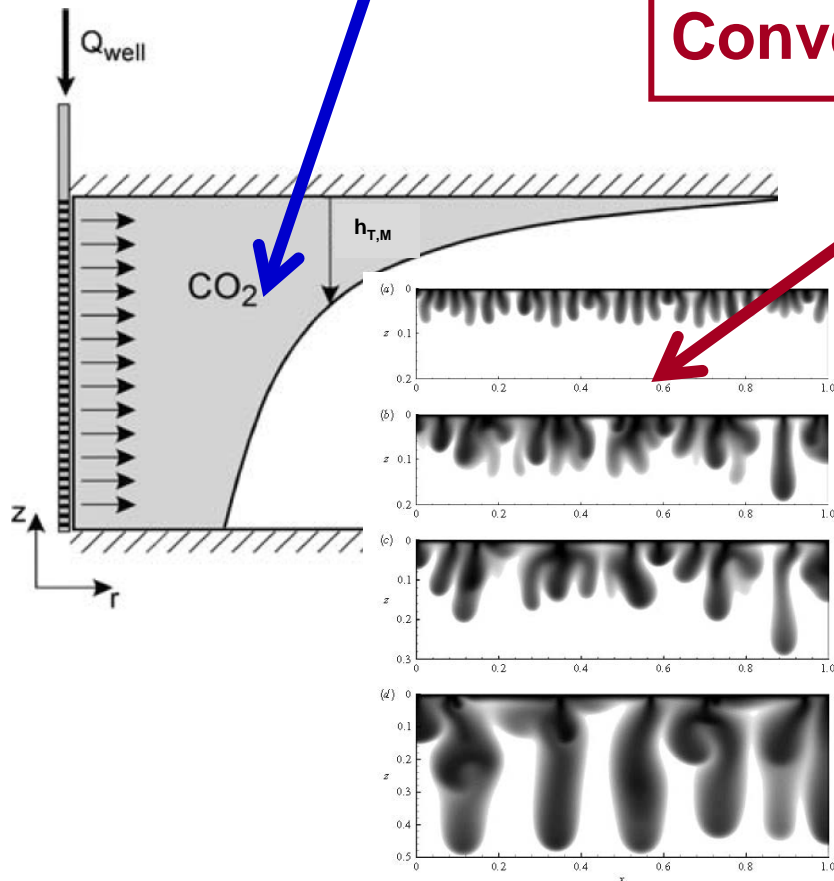
CO₂ Plume: Equilibrium Partitioning



Dissolution and Geochemistry

CO₂ Plume: Equilibrium Partitioning

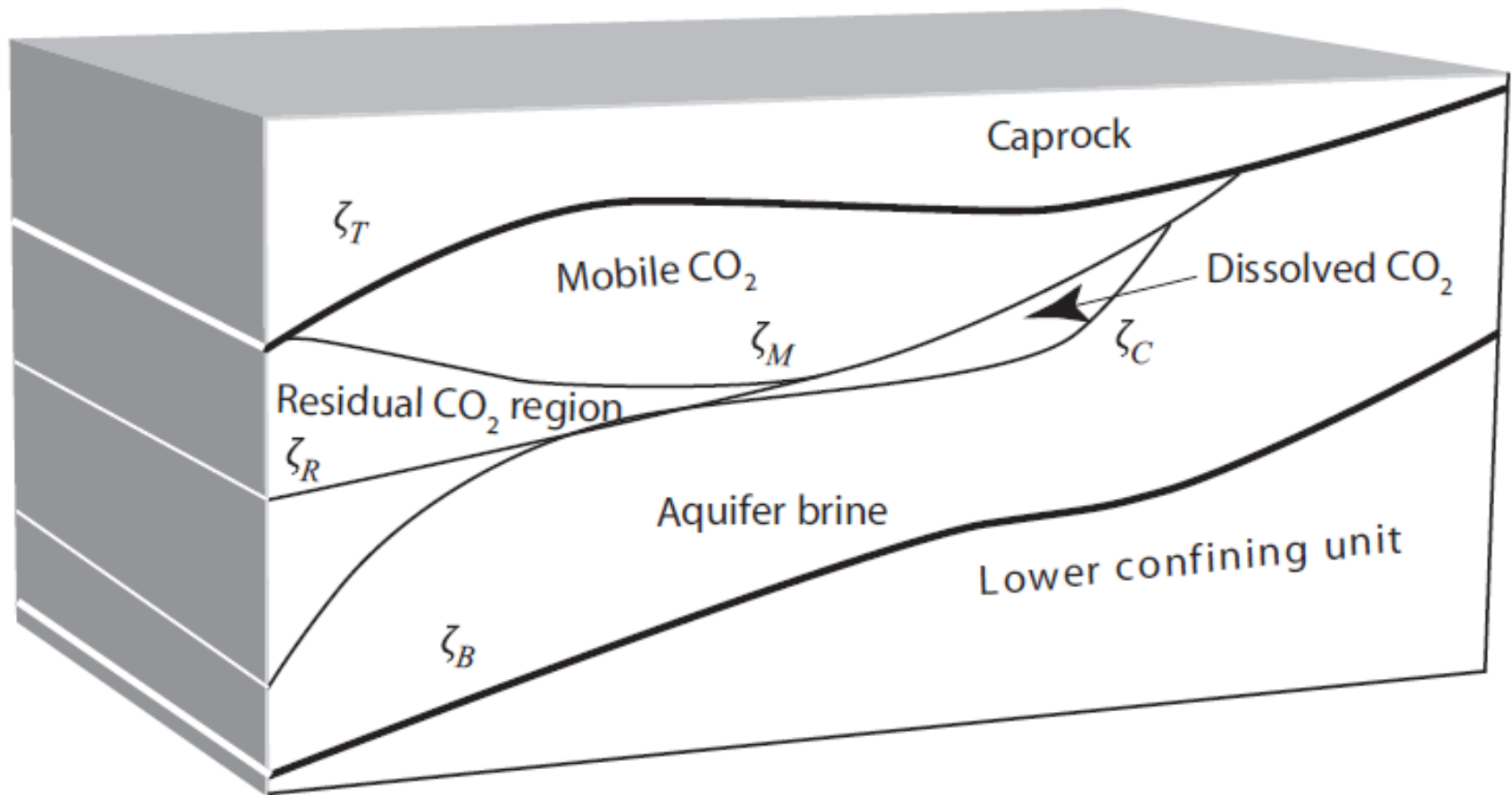
Dissolved CO₂ Transport in Brine: Convective Mixing



Advancement of dissolution fingers (Riaz et al. 05)



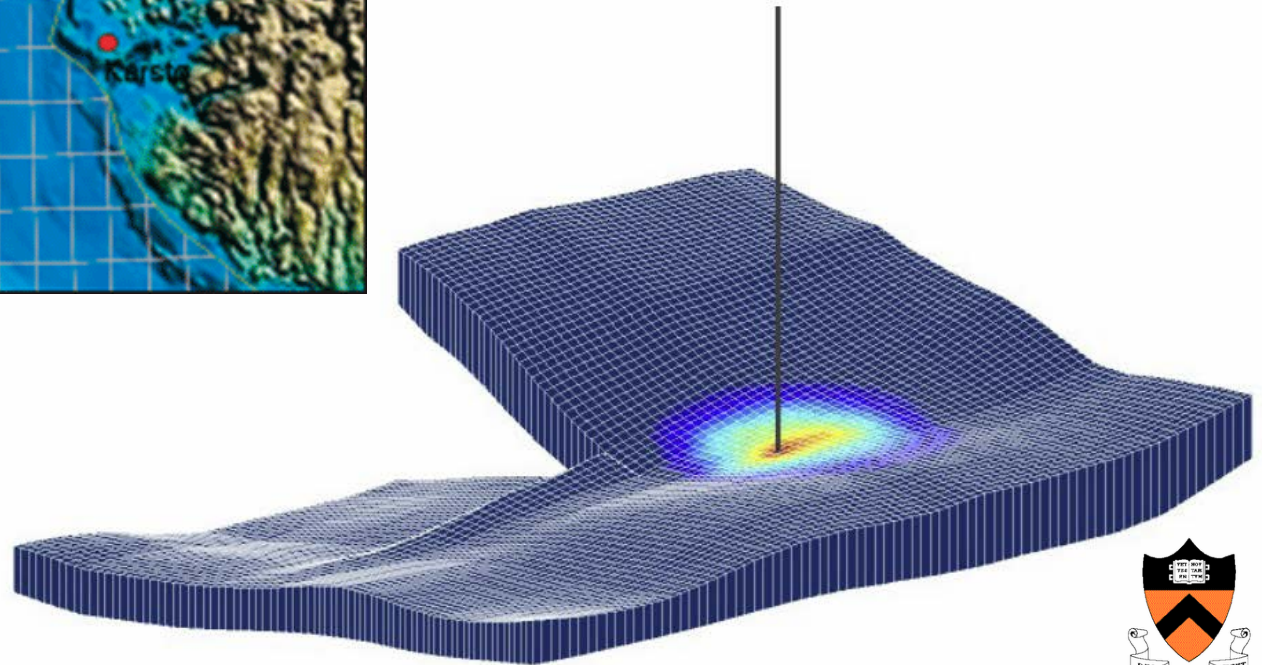
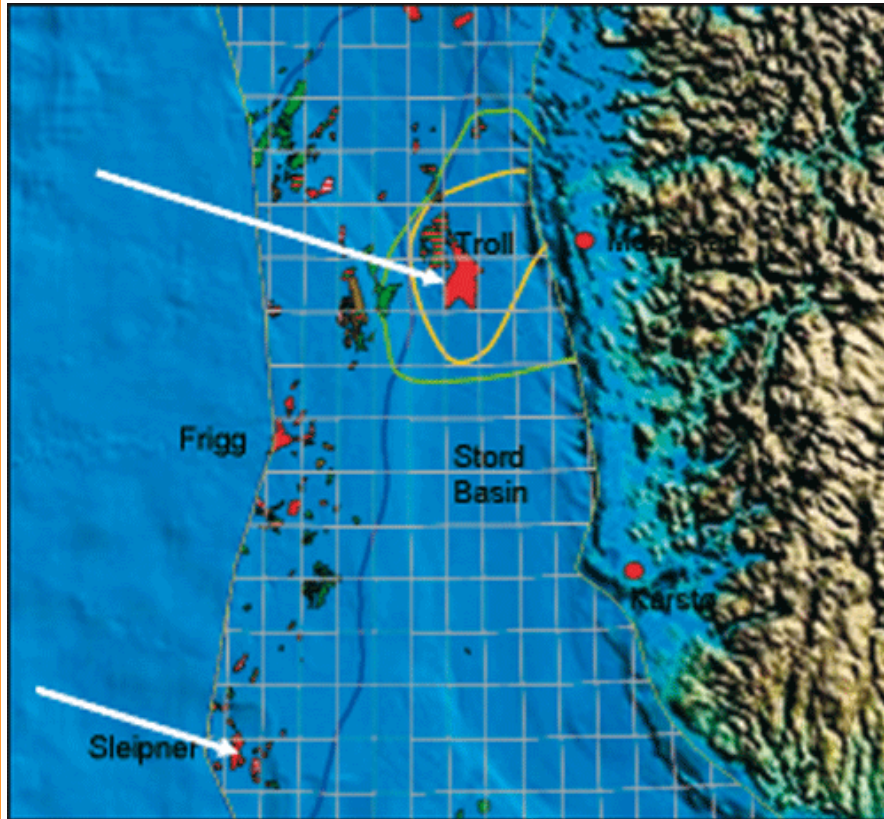
MODELS WITH CAPILLARY TRAPPING AND DISSOLUTION

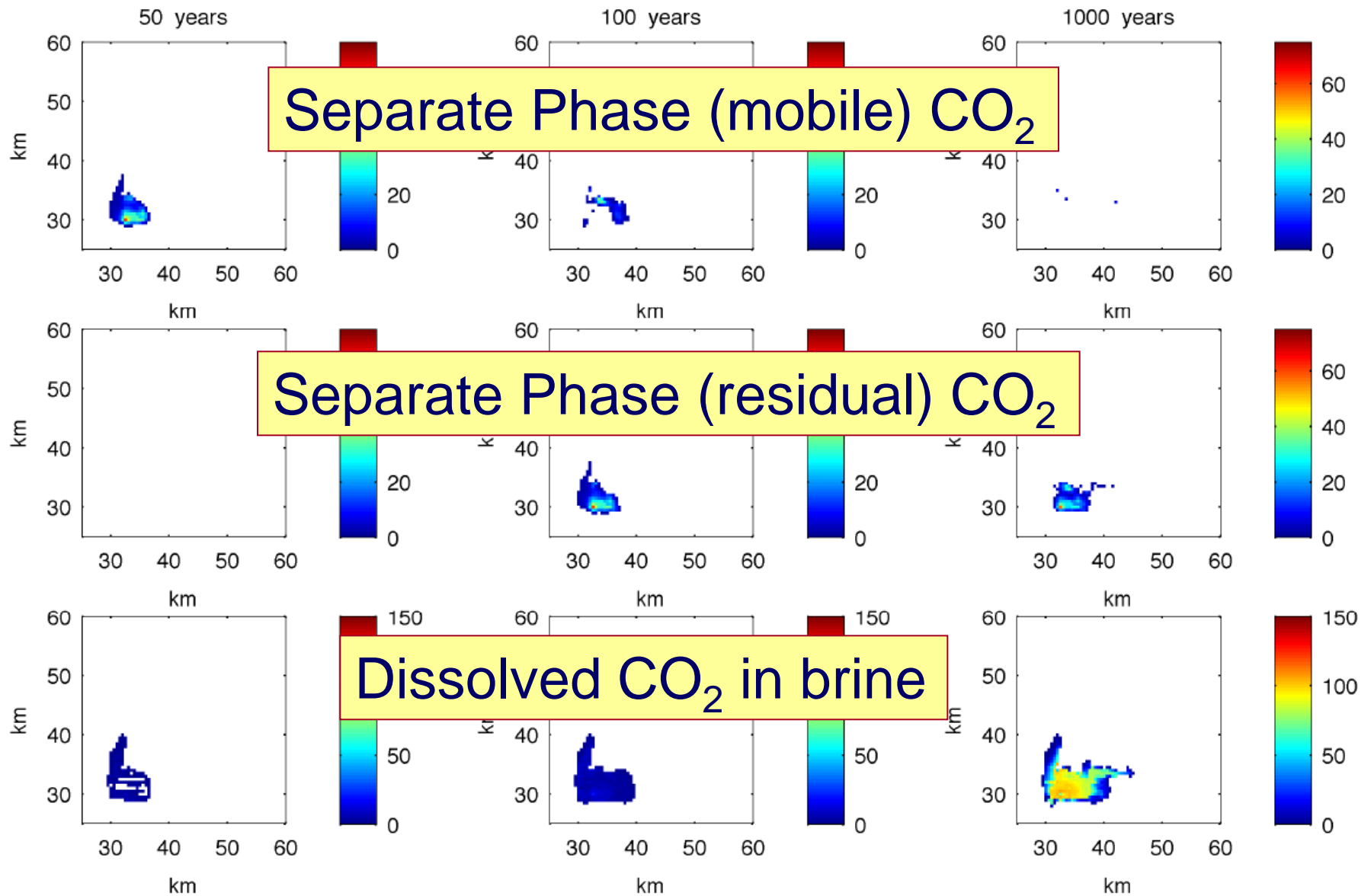


(See: Bandilla et al., 2013; Gasda et al., 2011, 2012;
Nordbotten and Celia, 2012)



LARGE-SCALE APPLICATION OF VE MODEL

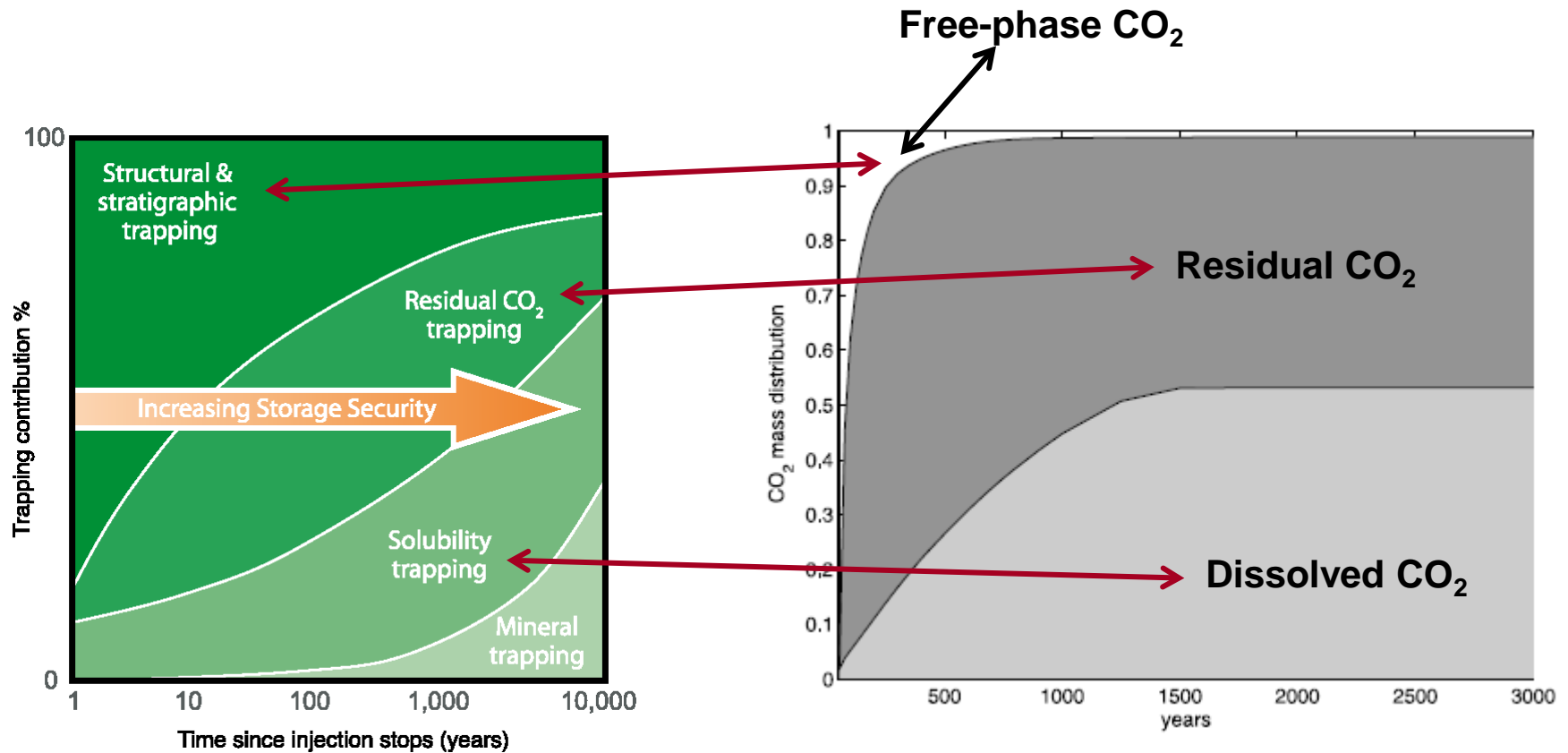




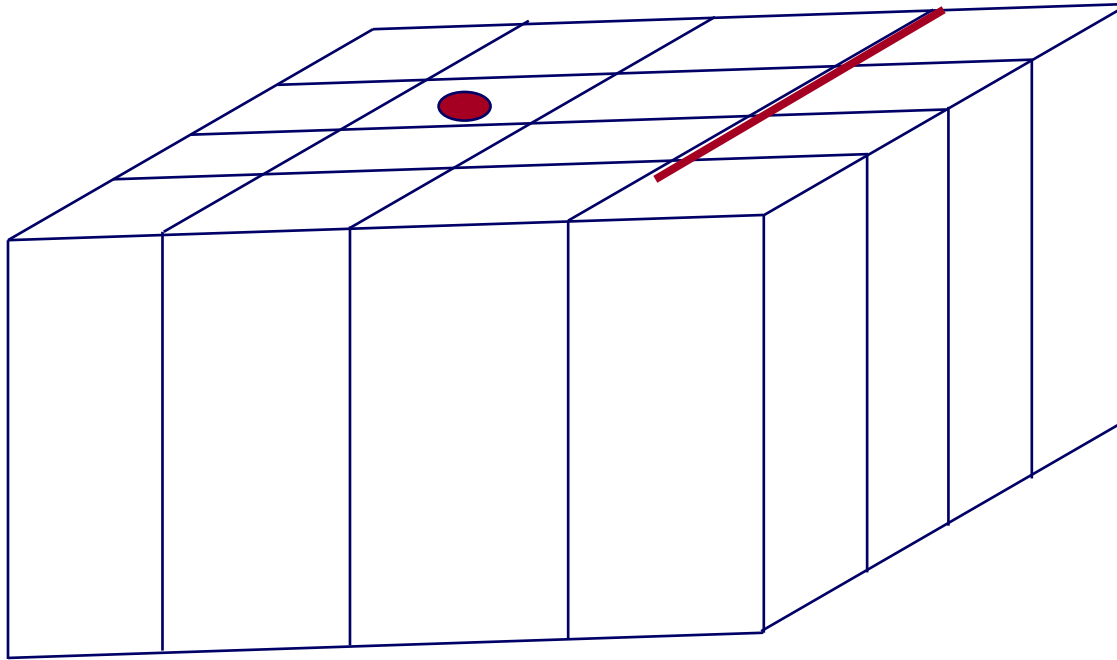
(See: Gasda et al., 2011, 2012)



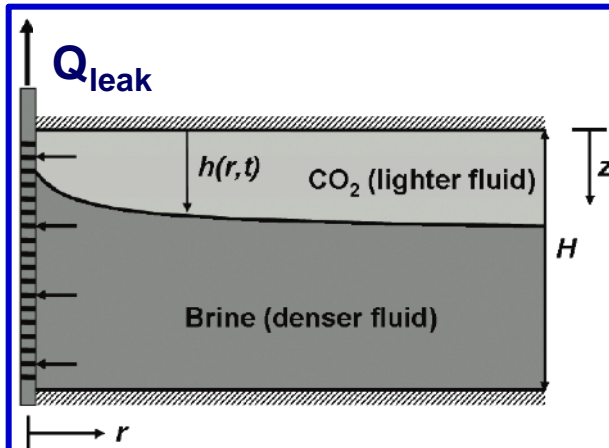
Long-term Predictions



Fault, Fractures, Wells, Leakage



**Modified
“Peaceman-type”
corrections**



$$\Gamma \lambda \frac{dh}{dx} + \frac{k'}{3} \left[-2\Gamma \lambda \frac{\left(\frac{dh}{dx}\right)^3}{1 + k' \left(\frac{dh}{dx}\right)^2} + \lambda Q'_d \left(\frac{d^2h}{dx^2} + \frac{1}{1-h} \left(\frac{dh}{dx}\right)^2 \right) + Q'_l \left(\frac{d^2h}{dx^2} - \frac{1}{h} \left(\frac{dh}{dx}\right)^2 \right) \right] = \frac{Q'_d \lambda}{1-h} - \frac{Q'_l}{h}.$$



CONCLUDING COMMENTS

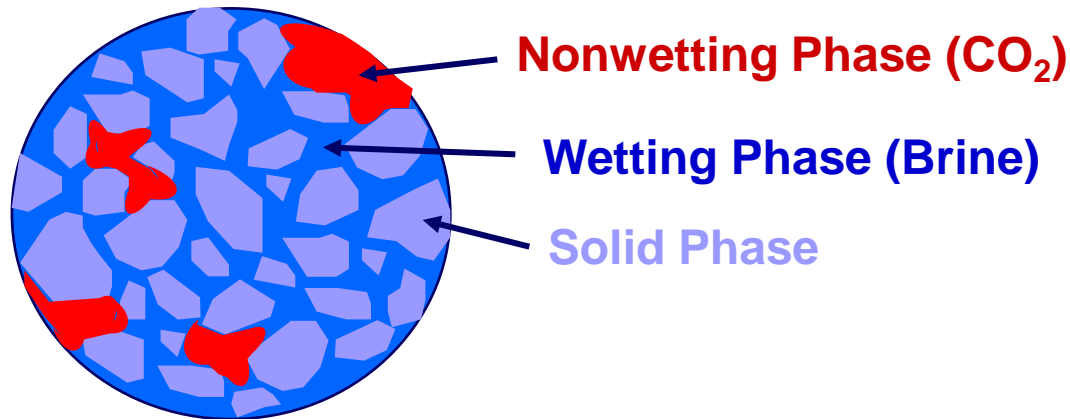
1. Vertically integrated models are often reasonable choices for practical calculations
2. A Multi-scale framework allows assumptions and representations across scales to be identified explicitly.
3. Most important processes can be included.
4. Extensions include complete hysteresis, thermal effects, geomechanics, and vertical dynamics.
5. Models should be compatible with the questions being asked and the available data.



MULTI-SCALE MODELS

Upscaling \longleftrightarrow Downscaling

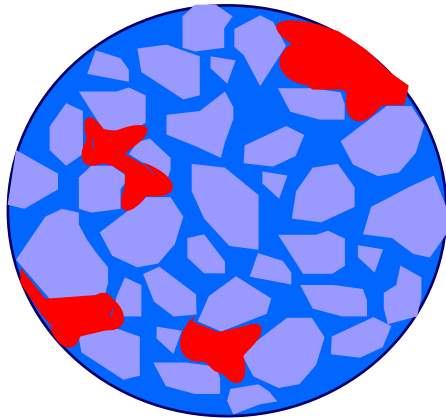
Compression \longleftrightarrow Reconstruction



MULTI-SCALE MODELS

Upscaling \longleftrightarrow Downscaling

Compression \longleftrightarrow Reconstruction



Compression

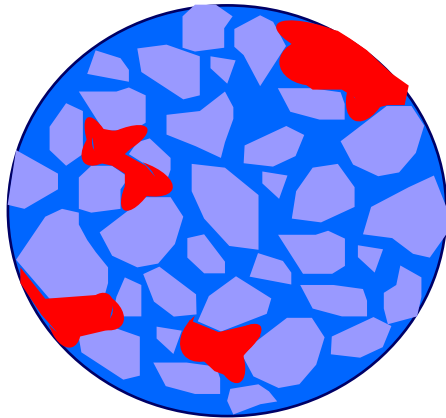


$$\varphi = \frac{V_{voids}}{V_{tot}}$$
$$s_{\alpha} = \frac{V_{\alpha}}{V_{voids}}$$

MULTI-SCALE MODELS

Upscaling \longleftrightarrow Downscaling

Compression \longleftrightarrow Reconstruction



Reconstruction



??

$$\varphi = \frac{V_{voids}}{V_{tot}}$$
$$s_{\alpha} = \frac{V_{\alpha}}{V_{voids}}$$